THE COEFFICIENTS OF FRACTIONAL PARENTAGE OF NUCLEAR SHELL MODEL

A.Deveikis, G.Kamuntavičius

Vytautas Magnus University, Kaunas 3000, Lithuania

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Abstract

A new procedure has been developed for the calculation of shell model coefficients of fractional parentage. This procedure is free from the numerical diagonalization, orthogonalization and even group theoretical antisymmetric states classification.

I. INTRODUCTION

New phenomena, obtained recently in nuclear physics (neutron - rich nuclei and neutron halo) cannot be described in shell- model approximation and require high - quality wave function. One of the most efficient methods for the construction of many - particle wave functions with well - defined permutational symmetry and exact quantum numbers (J - total angular momentum and T - isospin) is the iterative procedure for the calculation of coefficients of fractional parentage (CFP) developed in classical works [1,2]. However, due to the high degree of degeneracy of shell - model states, the set of exact quantum numbers in many cases is not rich enough to classify different antisymmetrical states of system.

The first method for classifying antisymmetrical states [3] involves the construction and diagonalization of the matrices representing the quadratic Casimir operators for the appropriate special unitary, orthogonal or symplectic groups. The real difficulty in such a case is finding the Casimir operator and knowing its eigenvalues.

For many applications the precise specification of the states is not required. It is merely sufficient that the states be orthogonal. The second method [4] uses the Redmond iteration technique in conjunction with numerical Schmidt orthogonalization or Grammian matrix diagonalization. Unfortunately, although this procedure can generate complete sets for large spaces, the buildup of numerical errors in the process of imposing orthonormality within the overcomplete set of antisymmetrical states causes many problems.

We shall here present a new and very simple method of CFP calculation, based on complete rejection of group - theoretical antisymmetrical shell model states classification and even of numerical diagonalization or orthogonalization.

II. DEFINITIONS AND NOTATIONS

Coefficients of fractional parentage are defined as the coefficients for the expansion of antisymmetrical wave - function in terms of the complete set of the vector - coupled parent states with a lower degree of antisymmetry. In the simplest case (one particle CFP) this expansion is:

$$\langle x_1,\ldots,x_{N-1},x_N|K\alpha JTM_JM_T\rangle = \sum_{\substack{\bar{K}\bar{\alpha}\bar{J}\bar{T}\\ \varepsilon_N\ell_N j_N}} \left\langle x_1,\ldots,x_{N-1};x_N|\left(\bar{K}\bar{\alpha}\bar{J}\bar{T};\varepsilon_N\ell_N j_N\right)JTM_JM_T\right\rangle \times$$
$$\times\left\langle \bar{K}\bar{\alpha}\bar{J}\bar{T};\varepsilon_N\ell_N j_N \parallel K\alpha JT\right\rangle \ .$$

Here one – particle variables are $x_i \equiv \mathbf{r}_i\sigma_i\tau_i$ (set of corresponding radius – vector, spin and isospin variables) and quantum numbers $\varepsilon_i\ell_i j_i$ (oscillator energy, orbital momentum and total momentum).

The corresponding set of many - particle state quantum numbers are K – configuration (it can consist of only one shell nucleons), α – all necessary additional quantum numbers and JT – exact quantum numbers. Semicolon means that the corresponding wave - function is fully antisymmetric with respect to interchanges among the nucleons variables, distributed in different sides of this sign. Notice the use of parentheses to represent angular momentum coupling. $\langle\ldots;\ldots\parallel\ldots\rangle$ is the coefficient of the fractional parentage identificator.

The expression given above is written down in $j-j$ coupling, but final results are not dependent on the coupling scheme.

To calculate coefficients of fractional parentage it is enough to calculate N - particle antisymmetrization operator matrix into the basis of right - hand functions (with a lower degree of antisymmetry). As usual, one assumes that all $(N-1)$ particle CFPs have been obtained at a previous stage. The antisymmetrizer

$$A \equiv A_{1,\ldots,N} = \frac{1}{N!} \sum_{P \in S_N} \delta_P P$$

is normalized such that $A^2 = A$ and could be presented as

$$A_{1,\ldots,N} = A_{1,\ldots,N-1} Y A_{1,\ldots,N-1} \ ,$$

where

$$Y = \frac{1}{N} \left\{ 1 - (N-1) P_{N-1,N} \right\} \ .$$

Here the operator $P_{N-1,N}$ simply interchanges the coordinates x_{N-1} and x_N. Because the above mentioned basis is antisymmetrical by $x_1, \ldots, x_{N-1}$ variables permutation, matrix $\mathbf{A}$ equals the matrix of a far simpler operator Y:

$$\left\langle \left(\bar{K} \bar{\alpha} \bar{J} \bar{T}, \varepsilon_N \ell_N j_N \right) JTM_J M_T | Y | \left(\bar{K}' \bar{\alpha}' \bar{J}' \bar{T}', \varepsilon'_N \ell'_N j'_N \right) JTM_J M_T \right\rangle$$

$$= \tfrac{1}{N} \left\{ \delta_{\bar{K},\bar{K}'} \delta_{\bar{\alpha},\bar{\alpha}'} \delta_{\bar{J},\bar{J}'} \delta_{\bar{T},\bar{T}'} \delta_{\varepsilon_N,\varepsilon'_N} \delta_{\ell_N,\ell'_N} \delta_{j_N,j'_N} \right.$$

$$+ (-1)^{j_N + j'_N + \bar{J} + \bar{T} + \bar{J}' + \bar{T}'} (N-1) [(2\bar{J}+1)(2\bar{T}+1)(2\bar{J}'+1)(2\bar{T}'+1)]^{\frac{1}{2}}$$

$$\times \sum_{\tilde{K}\tilde{\alpha}\tilde{J}\tilde{T}} \left\{ \begin{array}{cc} j'_N & \tilde{J} \bar{J} \\ j_N & J \bar{J}' \end{array} \right\} \left\{ \begin{array}{cc} \frac{1}{2} & \tilde{T} \bar{T} \\ \frac{1}{2} & T \bar{T}' \end{array} \right\} \left\langle \tilde{K} \tilde{\alpha} \tilde{J} \tilde{T}; \varepsilon'_N \ell'_N j'_N \parallel \bar{K} \bar{\alpha} \bar{J} \bar{T} \right\rangle$$

$$\left. \times \left\langle \tilde{K} \tilde{\alpha} \tilde{J} \tilde{T}; \varepsilon_N \ell_N j_N \parallel \bar{K}' \bar{\alpha}' \bar{J}' \bar{T}' \right\rangle \right\} \ .$$

$\mathbf{A}$ is the symmetrical real matrix – projection $(\mathbf{A}^+ = \mathbf{A} = \mathbf{A}^* \ , \ \mathbf{AA} = \mathbf{A})$. Its eigenvalues are only zeros and units, and the spectral decomposition [5] is

$$\mathbf{A}_{n\times n} = \tilde{\mathbf{F}}_{n\times r} \left(\tilde{\mathbf{F}}^+\right)_{r\times n} \ .$$

The subscripts indicate the dimension of the corresponding matrix. n equals the dimension of the basis, r – rank of matrix $\mathbf{A}$. Every column of $\tilde{\mathbf{F}}$ is eigenvector of matrix $\mathbf{A}$, corresponding to a unit eigenvalue. The normalization condition of eigenvectors is

$$\left(\tilde{\mathbf{F}}^+\right)_{r\times n} \cdot \tilde{\mathbf{F}}_{n\times r} = \mathbf{1}_{r\times r} \ .$$

The matrix elements of $\tilde{\mathbf{F}}$ are coefficients of fractional parentage [6].

III. NEW RESULTS

Condition $\mathbf{A}_{n\times n}\mathbf{A}_{n\times n} = \mathbf{A}_{n\times n}$ means that every $\mathbf{A}_{n\times n}$ column is its eigenvector with unit eigenvalue. However, they are not normalized and even orthogonal, and only r of them are linearly independent. The simplest method of CFP matrix calculation is based on the observation that the spectral decomposition of $\mathbf{A}$ is not defined uniquely. The possibility exists of a free choice of orthogonal matrix $\mathbf{G}_{r\times r}$ defined as

$$\mathbf{A} = \tilde{\mathbf{F}}\mathbf{G}\mathbf{G}^+\tilde{\mathbf{F}}^+ \equiv \mathbf{F}\mathbf{F}^+ \ ,$$

because

$$\mathbf{F}^+\mathbf{F} \equiv \mathbf{G}^+\tilde{\mathbf{F}}^+\tilde{\mathbf{F}}\mathbf{G} = \mathbf{G}^+\mathbf{G} = \mathbf{1} \ .$$

Orthogonal matrix has $r(r-1)/2$ free parameters, so we can choose it in a way which allows us to fix the corresponding number of $\mathbf{F}$ elements. The best choice is

$$F_{ij} = 0 \qquad \text{if} \quad 1 \le i < j \le r \ .$$

This means that the upper triangle of matrix $\mathbf{F}$ equals zero. In such a case we can obtain the solution of matrix equation $\mathbf{A} = \mathbf{F}\mathbf{F}^+$ in the following way. Starting with the well – known Redmond result [2] for the first row

$$F_{11}^2 = A_{11} \ , \quad F_{j1} = A_{1j}/F_{11} \ ,$$

we can present the following columns of $\mathbf{F}$ in the form:

$$F_{ii}^2 = A_{ii} - \sum_{k=1}^{i-1} F_{ik}^2 \ ,$$
$$F_{ji} = \frac{1}{F_{ii}} \left\{ A_{ij} - \sum_{k=1}^{i-1} F_{ik} F_{jk} \right\}$$

for every value of $i = 2, 3, ..., r$ and the corresponding set of $j = i+1, i+2, ..., n$. Positive values of F_{ii} are convenient, because the overall sign of CFP vector is arbitrary. Obviously, if $\mathbf{F}$ is constructed in this way, it fulfils the condition $\mathbf{F}^+\mathbf{F} = \mathbf{1}$.

So to obtain the spectral decomposition of an antisymmetrization operator matrix with rank r, it is enough to calculate only the r linearly independent rows of this matrix. The calculation begins with the first matrix $\mathbf{A}$ row. If

$$A_{11} = 0 \ ,$$

then every element of the first row and the first column equals zero, because by definition

$$A_{11} = \sum_{j=1}^{n} A_{1j}^2 \ .$$

This means that the corresponding basic function is not presented in fractional parentage expansion (it may be, that it has some hidden symmetry, wrong quantum numbers, etc.). Such a function has to be omitted from all the expansions in every case, when $A_{ii} = 0$ appears. Because matrix $\mathbf{A}$ is symmetrical, every next row calculation starts from diagonal element (A_{ll}). Then it is necessary to find the corresponding minor $(\mathbf{A}_{l\times l})$ determinant value. If it equals zero, l–th row is linearly dependent on $(l-1)$ the just calculated ones, because this determinant equals calculated rows Grammian:

$$A_{ij} = \sum_{k=1}^{n} A_{ik} A_{jk} \ .$$

Only in the case when $A_{ll} \neq 0$ and $det\ \mathbf{A}_{l\times l} \neq 0$, is it worth finishing the l–th row calculation. Because $\mathbf{A}$ is a projection by definition, the necessary number (n) of basic states is included only in the case when the condition is fulfilled:

$$\sum_{j=1}^{n} A_{lj}^2 = A_{ll} \ .$$

It is also useful to know the sum of matrix **A** diagonal elements, because

$$Sp\,\mathbf{A} = r \ .$$

The expansions which have been presented allow after the calculation of every matrix element of **A** (A_{ij}) to obtain the corresponding CFP (F_{ji}).

So the calculation of one linearly independent row of **A** gives us the coefficients for one antisymmetrical state expansion (one column of CFP matrix). Columns of **F** can be numbered by the positive integer numbers $\alpha = 1, 2, \ldots, r$. In this definition, α also equals the number of zeros present in the corresponding column plus one.

IV. COMPUTATION RESULTS

The general formalism described above was implemented in computer code to generate complete sets of CFP for the $j = 1/2, 3/2, 5/2$ shells in isospin formalism. Angular momentum coupling and antisymmetrization are orthogonal transformations, so is possible precise arithmetic with quantities no more sophisticated as square root of integer number. The CFP computational procedure required four different types of arithmetics:

- algebraic and relation operations between fractions composed of 16 - bit integer numbers for operating with quantities like angular momentum.
- square root of 64 - bit integer numbers.
- algebraic and relation operations between numbers represented in the form $n/m/\sqrt{k}$, where n,m,k are 64 - bit integer numbers for both middle scale and 6j coefficient calculations.
- algebraic and relation operations between numbers represented in the form $n/m/\sqrt{k}$, where n,m,k are arbitrary length integer numbers accomplished as variable long vector

with prescribed position weight for large scale calculations in evaluation **A** and **F** matrices. Orbit $j = 5/2$ was calculated with 20 - position vectors and position weight equal to 1000.

As a preliminary step complete enumeration of the states in isospin formalism was carried out. By means of combinatorial calculations all JT and number of states with the same JT were found. This enable find out all permited CFP and to characterized them uniquely by means of parent and daugther states. Results for the $j = 5/2$ nuclear shell are presented in the table.

N	T	n(J)m						
2	0	1(1)1	1(3)1	1(5)1				
	1	1(0)1	1(2)1	1(4)1				
3	1/2	2(1/2)1	4(3/2)1	6(5/2)2	5(7/2)2	4(9/2)1	3(11/2)1	2(13/2)1
	3/2	2(3/2)1	3(5/2)1	2(9/2)1				
4	0	2(0)2	7(2)3	8(3)1	8(4)3	7(5)1	5(6)2	2(8)1
	1	7(1)2	10(2)2	11(3)3	11(4)2	9(5)2	6(6)1	4(7)1
	2	1(0)1	3(2)1	3(4)1				
5	1/2	9(1/2)2	16(3/2)3	21(5/2)4	22(7/2)4	21(9/2)4	17(11/2)3	13(13/2)2
		8(15/2)1	5(17/2)1					
	3/2	6(1/2)1	11(3/2)2	14(5/2)2	14(7/2)2	13(9/2)2	10(11/2)1	7(13/2)1
	5/2	3(5/2)1						
6	0	11(1)3	17(2)1	20(3)5	20(4)2	18(5)3	15(6)2	11(7)2
		4(9)1						
	1	6(0)2	17(1)1	26(2)5	30(3)3	30(4)5	26(5)2	21(6)3
		15(7)1	9(8)1					
	2	7(1)1	10(2)1	11(3)1	11(4)1	9(5)1		
	3	1(0)1						

7	1/2	14(1/2)2	25(3/2)3	32(5/2)4	35(7/2)4	34(9/2)4	29(11/2)3	22(13/2)2
		15(15/2)1	10(17/2)1					
	3/2	10(1/2)1	18(3/2)2	23(5/2)2	24(7/2)2	23(9/2)2	18(11/2)1	14(13/2)1
	5/2	6(5/2)1						
8	0	4(0)2	17(2)3	20(3)1	20(4)3	18(5)1	15(6)2	7(8)1
	1	17(1)2	26(2)2	30(3)3	30(4)2	26(5)2	21(6)1	15(7)1
	2	3(0)1	10(2)1	11(4)1				
9	1/2	9(1/2)1	16(3/2)1	21(5/2)2	22(7/2)2	21(9/2)1	17(11/2)1	13(13/2)1
	3/2	11(3/2)1	14(5/2)1	13(9/2)1				
10	0	5(1)1	8(3)1	7(5)1				
	1	3(0)1	10(2)1	11(4)1				
11	1/2	6(5/2)1						
12	0	1(0)1						

First column contains nucleon number N in the shell, second stands for total isospin T, last column gives total J and two additional numbers: n - CFP number for specified JT (the dimension of corresponding A matrix); m - stands for number of states with the same JT (the rank of a corresponding A matrix). Thus we can have $n \times m$ CFP with the same JT. Though generally $j = 5/2$ nuclear shell has 3359 CFP, computational method determines $m(m-1)/2$ zeros by zeroing **F** matrix upper right corner. This gives 141 zeros in complete CFP set. Actual number of CFP equal to zero is 328 due possible nonincounted symmetries.

To illustrate the evaluation of the CFP consider N=4 state with J = 6, T = 0. As follows from the combinatorial calculation in this case **A** matrix dimension is 5 and rank 2.

$$\mathbf{A}_4^{[6,0]} = \begin{pmatrix} \frac{5}{12} & \frac{7}{12\sqrt{33}} & \frac{14}{3\sqrt{462}} & \frac{-21}{2\sqrt{2002}} & \frac{28}{\sqrt{6006}} \\ & \frac{53}{396} & \frac{-56}{99\sqrt{14}} & \frac{-147}{22\sqrt{546}} & \frac{14}{33\sqrt{182}} \\ & & \frac{49}{99} & \frac{21}{11\sqrt{39}} & \frac{35}{33\sqrt{13}} \\ & & & \frac{175}{286} & \frac{-21}{143\sqrt{3}} \\ & & & & \frac{49}{143} \end{pmatrix}$$

Computed matrix is matrix projection, its rows and columns are labeled by CFP left - hand bracket indices. **A** matrix spectral decomposition gives **F** matrix, which has 2 columns(as predicted by combinatorial calculation) and contains CFP as matrix elements. To facilitate comprehension **F** matrix is displayed in one column.

$$\langle 3(2): \ 7/2,1/2;5/2,1/2||4(2):6,0\rangle = \frac{5}{2\sqrt{15}}$$
$$\langle 3(1): \ 7/2,1/2;5/2,1/2||4(2):6,0\rangle = \frac{7}{6\sqrt{55}}$$
$$\langle 3(1): \ 9/2,1/2;5/2,1/2||4(2):6,0\rangle = \frac{28}{3\sqrt{770}}$$
$$\langle 3(1):11/2,1/2;5/2,1/2||4(2):6,0\rangle = \frac{-63}{\sqrt{30030}}$$
$$\langle 3(1):13/2,1/2;5/2,1/2||4(2):6,0\rangle = \frac{56}{\sqrt{10010}}$$
$$\langle 3(2): \ 7/2,1/2;5/2,1/2||4(1):6,0\rangle = 0$$
$$\langle 3(1): \ 7/2,1/2;5/2,1/2||4(1):6,0\rangle = \frac{6}{\sqrt{330}}$$
$$\langle 3(1): \ 9/2,1/2;5/2,1/2||4(1):6,0\rangle = \frac{-21}{\sqrt{1155}}$$
$$\langle 3(1):11/2,1/2;5/2,1/2||4(1):6,0\rangle = \frac{-49}{\sqrt{5005}}$$
$$\langle 3(1):13/2,1/2;5/2,1/2||4(1):6,0\rangle = \frac{-21}{\sqrt{15015}}$$

CFP are denoted $\langle \bar{N}(\bar{\alpha}) : \bar{J},\bar{T};j,t||N(\alpha) : J,T\rangle$. First number in the bracket is $N-1$, second number closed in parentheses stands for parent state number with the same total angular momentum $\bar{J}$ and isospin $\bar{T}$, shell's j and t stands after semicolon. The same is for daughter state in the right - hand. Columns of matrix **F** form orthonormalized sets of CFP: columns with the same α are normalized to unit and orthogonal.

V. CONCLUSIONS

The suggested method of CFP calculation is not dependent on a coupling scheme and configuration complexity. It is the same in every case. So, it is useful in the description of highly excited states, when we try to investigate more interesting phenomena. The method is useful

for intrinsic CFP calculation, when the system centrum of mass state is under control in every antisymmetrical basic function. It is for this reason that we have introduced the original CFP abbreviation and defined the procedure for arbitrary configuration. How about possible numerical instabilities, we have developed arithmetic, which allows calculations without approximations. Numbers are represented in the form: $n/m/\sqrt{k}$, where n,m,k are integer numbers, and all calculations are made with numbers in this form. Our computational experience shows that method has high accuracy, therefore real numbers are insufficient. We have used 25 Mhz AT - 386 for calculation of CFP of the nuclear shell j = 5/2 and it take us about 20 hours.

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